Amendments to the Claims:

This listing of claims replaces all prior versions and listings of claims in the application:

Listing of Claims:

1. (currently amended) A method of constructing a modular computational model for predicting one or more therapeutic properties of a chemical compound, comprising:

obtaining a first set of data describing the interaction between each training compound of a first set of training compounds and a first interaction partner, wherein the first set of data is obtained experimentally using a high throughput instrument; and

using the first set of data, along with data about the chemical structures and/or physical properties thereof of the first set of training compounds and, optionally, data about the three dimensional structure and/or physical properties thereof of the first interaction partner, to construct a computer-based first module that uses data about the chemical structures and/or physical properties thereof of chemical compounds to predict values describing the interaction between a chemical compound and the first interaction partner, wherein the predicted values are the same type of data as the data contained in the first set of data;

thereby constructing a single module modular computational model for predicting one or more therapeutic properties of a chemical compound.

2. (canceled)

3. (previously presented) The method of claim 2, wherein the high throughput instrument is a multi-channel or multi-cell calorimeter.

4. (previously presented) The method of claim 1, wherein the first set of data includes measurements of enthalpy, ΔH.

5. (previously presented) The method of claim 4, wherein the first set of data includes distinct measurements of enthalpy, ΔH, entropy, ΔS, and free energy, ΔG.

6. (previously presented) The method of claim 1, further comprising:

obtaining a second set of data describing the interaction between each training compound of a second set of training compounds and a second interaction partner;

using the second set of data, along with data about the chemical structures and/or physical properties thereof of the second set of training compounds and, optionally, data about the three dimensional structure and/or physical properties thereof of the second interaction partner, to construct a second module that uses data about the chemical structures and/or physical properties thereof of chemical compounds to predict values describing the interaction between a chemical compound and the second interaction partner, wherein the predicted values are of the same type of data as the data contained in the second set of data;

thereby constructing a two module modular computational model for predicting one or more therapeutic properties of a chemical compound.

7. (previously presented) The method of claim 6, wherein at least one of the modules predicts therapeutic property values that are relevant to the therapeutic potency of compounds.

8. (currently amended) The method of claim 7, wherein the module that predicts values relevant to therapeutic potency is a ~~4D-QSAR~~ four dimensional quantitative structure-activity relationship (4D-QSAR) model.

9. (previously presented) The method of claim 7, wherein the interaction partner of the module that predicts values relevant to therapeutic potency comprises a protein.

10. (previously presented) The method of claim 9, wherein the protein is a hormone.

11. (currently amended) The method of claim 6, wherein at least one of the modules predicts therapeutic property values that are relevant to one or more ~~ADMET~~ absorption, distribution, metabolism, excretion or toxicological (ADMET) properties of compounds.

12. (currently amended) The method of claim 11, wherein the module that predicts therapeutic values relevant to one or more ADMET properties of compounds is a membrane interaction quantitative structure-activity relationship (MI-QSAR) ~~MI-QSAR~~ model.

13. (previously presented) The method of claim 11, wherein the interaction partner of the module that predicts therapeutic property values that are relevant to one or more ADMET properties of compounds comprises a membrane having properties identical or consistent with biological membranes.

14. (previously presented) The method of claim 13, wherein the membrane is part of a Caco-2 cell.

15. (previously presented) The method of claim 6, wherein at least one of the modules predicts therapeutic property values that are relevant to the therapeutic potency of compounds, and wherein at least one the modules predicts therapeutic property values that are relevant to one or more ADMET properties of compounds.

16. (previously presented) The method of claim 6, further comprising:

obtaining a third set of data describing the interaction between each training compound of a third set of training compounds and a third interaction partner;

using the third set of data, along with data about the chemical structures and/or physical properties thereof of the third set of training compounds and, optionally, data about the three dimensional structure and/or physical properties thereof of the third interaction partner, to construct a third module that uses data about the chemical structures and/or physical properties thereof of chemical compounds to predict values describing the interaction between a chemical compound and the third interaction partner, wherein the predicted values are of the same type of data as the data contained in the second set of data;

thereby constructing a three module modular computational model for predicting one or more therapeutic properties of a chemical compound.

17. (currently amended) The method of claim 16, wherein at least one of the wherein at least one of the modules predicts therapeutic property values that are relevant to the therapeutic potency of compounds, wherein at least one of the other the modules predicts therapeutic property values that are relevant to one or more ADMET properties of compounds, and wherein the final module predicts therapeutic property values distinct ~~form~~ from the therapeutic property predictions of the other two modules.

18. (withdrawn) A method of evaluating a plurality of test structures for one or more therapeutic properties, comprising:

a) providing a first modular computational model;

b) providing the chemical structure and/or physical properties thereof for all or a part of each member of the plurality of test structures;

c) applying the first modular computational model to each member of the plurality of test structures to obtain a first set of predicted values describing the interaction between each member of the plurality of test structures and one or more interaction partners; and optionally analyzing the values by:

d) comparing the predicted values from the first set of predicted values with one or more reference values; or

e) ranking the predicted values from the first set of predicted values,

thereby evaluating one or more therapeutic properties of the plurality of test structures.

19. (withdrawn) The method of claim 18, wherein the first modular computational model includes at least two modules.

20. (withdrawn) The method of claim 18, wherein at least one of the modules of the modular computational model makes predictions relevant to the therapeutic potency of test structures.

21. (withdrawn) The method of claim 20, wherein the module that makes predictions relevant to the therapeutic potency of test structures is a 4D-QSAR model.

22. (withdrawn) The method of claim 21, wherein the 4D-QSAR model predicts enthalpy (ΔH) values.

23. (withdrawn) The method of claim 18, wherein at least one of the modules of the modular computational model makes predictions relevant to one or more ADMET properties of compounds.

24. (withdrawn) The method of claim 23, wherein the module that makes predictions relevant to one or more ADMET properties is a MI-QSAR model.

25. (withdrawn) The method of claim 18, wherein at least one of the modules predicts therapeutic property values that are relevant to the therapeutic potency of compounds, and wherein at least one the modules predicts therapeutic property values that are relevant to one or more ADMET properties of compounds.

26. (withdrawn) The method of claim 25, wherein the plurality of test structures is ranked with respect to both therapeutic potency and one or more ADMET properties.

27. (withdrawn) The method of claim 26, wherein a subset of the test structures are identified as having a high rank with respect to both therapeutic potency and one or more desirable ADMET properties.

28. (withdrawn) The method of claim 18 further comprising a computer readable record of at least some of the pharmaceutical properties predictions generated by evaluation of the plurality of test structures.